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Characterization of barycenters in the Wasserstein space by averaging optimal transport maps

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Abstract

This paper is concerned by the study of barycenters for random probability measures in the Wasserstein space. Using a duality argument, we give a precise characterization of the population barycenter for various parametric classes of random probability measures with compact support. In particular, we make a connection between averaging in the Wasserstein space as introduced in Agueh and Carlier [2], and taking the expectation of optimal transport maps with respect to a fixed reference measure. We also discuss the usefulness of this approach in statistics for the analysis of deformable models in signal and image processing. In this setting, the problem of estimating a population barycenter from n independent and identically distributed random probability measures is also considered.

Keywords: Wasserstein space; Empirical and population barycenters; Fréchet mean; Convergence of random variables; Optimal transport; Duality; Curve and image warping; Deformable models.
AMS classifications: Primary 62G05; secondary 49J40.

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1 Introduction

In this paper, we consider the problem of characterizing the barycenter of random probability measures on $\mathbb{R}^d$. The set of Radon probability measures endowed with the 2-Wasserstein distance is not an Euclidean space. Consequently, to define a notion of barycenter for random probability measures, it is natural to use the notion of Fréchet mean [22] that is an extension of the usual Euclidean barycenter to non-linear spaces endowed with non-Euclidean metrics. If $\mathbf{Y}$ denotes a random variable with distribution $\mathbb{P}$ taking its value in a metric space $(\mathcal{M}, d_{\mathcal{M}})$, then a Fréchet

mean (not necessarily unique) of the distribution $\mathbb{P}$ is a point $m^* \in \mathcal{M}$ that is a global minimum (if any) of the functional

$$J(m) = \frac{1}{2}\int_{\mathcal{M}} d^2_{\mathcal{M}}(m, y) d\mathbb{P}(y) \quad \text{i.e.} \quad m^* \in \arg\min_{m\in\mathcal{M}} J(m).$$

In this paper, a Fréchet mean of a random variable $\mathbf{Y}$ with distribution $\mathbb{P}$ will be also called a barycenter. An empirical Fréchet mean of an independent and identically distributed (iid) sample $\mathbf{Y}_1, \ldots, \mathbf{Y}_n$ of distribution $\mathbb{P}$ is

$$\bar{\mathbf{Y}}_n \in \arg\min_{m\in\mathcal{M}} \frac{1}{n}\sum_{j=1}^{n} \frac{1}{2} d^2_{\mathcal{M}}(m, \mathbf{Y}_j).$$

For random variables belonging to nonlinear metric spaces, a well-known example is the computation of the mean of a set of planar shapes in the Kendall's shape space [30] that leads to the Procrustean means studied in [24]. Many properties of the Fréchet mean in finite dimensional Riemannian manifolds (such as consistency and uniqueness) have been investigated in [1, 7, 9, 10, 29]. For random variables taking their value in metric spaces of nonpositive curvature (NPC), a detailed study of various properties of their barycenter can be found in [38]. However, there is not so much work on Fréchet means in infinite dimensional metric spaces that do not satisfy the global NPC property as defined in [38].

1.1 A parametric class of random probability measures

In this paper, we consider the case where $\mathbf{Y} = \boldsymbol{\mu}$ is a random probability measure belonging to the 2-Wasserstein space on a compact set Ω of $\mathbb{R}^d$. In this work, we consider the following parametric class of random probability measures. Let $\mathcal{M}_+(\Omega)$ be the set of Radon probability measures on Ω endowed with the 2-Wasserstein distance d_{W_2} between two probability measures. Let $\Phi : (\mathbb{R}^p, \mathcal{B}(\mathbb{R}^p)) \to (\mathcal{M}_+(\Omega), \mathcal{B}(\mathcal{M}_+(\Omega))$ be a measurable mapping, where $\mathcal{B}(\mathbb{R}^p)$ is the Borel σ-algebra of $\mathbb{R}^p$ and $\mathcal{B}(\mathcal{M}_+(\Omega))$ is the Borel σ-algebra generated by the topology induced by the distance d_{W_2}. For a compact subset Θ of $\mathbb{R}^p$ (with $p \geq 1$), we consider the parametric set of probability measures $\{\mu_\theta = \Phi(\theta),\ \theta \in \Theta\}$. Futhermore, we assume that, for any $\theta \in \Theta$, the measure $\mu_\theta = \Phi(\theta) \in \mathcal{M}_+(\Omega)$ admits a density with respect to the Lebesgue measure on $\mathbb{R}^d$. It follows that if $\boldsymbol{\theta} \in \mathbb{R}^p$ is a random vector with distribution $\mathbb{P}_\Theta$ admitting a density $g : \Theta \to \mathbb{R}_+$, then $\mu_{\boldsymbol{\theta}} = \Phi(\boldsymbol{\theta})$ is a random probability measure with distribution $\mathbb{P}_g$ on $(\mathcal{M}_+(\Omega), \mathcal{B}(\mathcal{M}_+(\Omega))$ that is the push-forward measure defined by

$$\mathbb{P}_g(B) = \mathbb{P}_\Theta(\Phi^{-1}(B)), \text{ for any } B \in \mathcal{B}(\mathcal{M}_+(\Omega)). \tag{1.1}$$

In this paper, we propose to study some properties of the barycenter μ^* of $\mu_{\boldsymbol{\theta}}$ defined as the following Fréchet mean

$$\mu^* = \arg\min_{\nu\in\mathcal{M}_+(\Omega)} J(\nu), \tag{1.2}$$

where

$$J(\nu) = \int_{\mathcal{M}_+(\Omega)} \frac{1}{2} d^2_{W_2}(\nu, \mu) d\mathbb{P}_g(\mu) = \mathbb{E}\left(\frac{1}{2} d^2_{W_2}(\nu, \mu_{\boldsymbol{\theta}})\right) = \int_\Theta \frac{1}{2} d^2_{W_2}(\nu, \mu_\theta) g(\theta) d\theta,\ \nu \in \mathcal{M}_+(\Omega).$$

If it exists and is unique, the measure μ^* will be referred to as the population barycenter of the random measure $\mu_{\boldsymbol{\theta}}$ with distribution $\mathbb{P}_g$.

The empirical counterpart of μ^* is the barycenter $\bar{\boldsymbol{\mu}}_n$ defined as

$$\bar{\boldsymbol{\mu}}_n \quad = \quad \underset{\nu \in \mathcal{M}_+(\Omega)}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \frac{1}{2} d^2_{W_2}(\nu, \mu_{\boldsymbol{\theta}_i}), \tag{1.3}$$

where $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_n$ are iid random vectors in Θ with density g.

1.2 Main results of the paper

The main contribution of this paper is to give an explicit characterization of the population barycenter μ^* that can be (informally) stated as follows: let $\mu_0 \in \mathcal{M}_+(\Omega)$ be a fixed reference measure that is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}^d$, and let $T_{\boldsymbol{\theta}} : \Omega \to \Omega$ be the optimal mapping to transport μ_0 onto $\mu_{\boldsymbol{\theta}}$ (i.e. $\mu_{\boldsymbol{\theta}} = T_{\boldsymbol{\theta}} \# \mu_0$, where $T_{\boldsymbol{\theta}} \# \mu_0$ denotes the push-forward of the measure μ_0 through the mapping $T_{\boldsymbol{\theta}}$). If $\mathbb{E}(T_{\boldsymbol{\theta}}(x)) = x$ for all $x \in \Omega$, then μ_0 is equal to the population barycenter μ^*, and one has that

$$\inf_{\nu \in \mathcal{M}_+(\Omega)} J(\nu) = \frac{1}{2} \int_{\Omega} \mathbb{E}\left(|T_{\boldsymbol{\theta}}(x) - x|^2\right) d\mu^*(x) = \frac{1}{2} \int_{\Omega} \int_{\Theta} \left(|T_{\theta}(x) - x|^2\right) g(\theta) d\theta d\mu^*(x).$$

This result can also be written in the form $\mu^* = \bar{T} \# \mu_0$, where $\bar{T} = \mathbb{E}(T_{\boldsymbol{\theta}})$ is the mapping defined by $\bar{T}(x) = \mathbb{E}(T_{\boldsymbol{\theta}}(x))$, for all $x \in \Omega$. This suggests that averaging in the Wasserstein space may amount to take the expectation (in the usual sense) of the optimal transport map $T_{\boldsymbol{\theta}}$ with respect to a fixed reference measure μ_0. However, this result is generally not true if $\mathbb{E}(T_{\boldsymbol{\theta}}) \neq I$, where $I = \Omega \to \Omega$ denotes the identity mapping. Nevertheless, we propose to consider sufficient conditions (beyond the case $\mathbb{E}(T_{\boldsymbol{\theta}}) = I$) ensuring that

$$\mu^* = \bar{T} \# \mu_0, \text{ where } \bar{T} = \mathbb{E}(T_{\boldsymbol{\theta}}). \tag{1.4}$$

To the best of our knowledge, such a result on the population barycenter in the 2-Wasserstein space is new. A similar result has been established in [15] for the empirical barycenter, namely that

$$\bar{\boldsymbol{\mu}}_n = \left(\frac{1}{n} \sum_{i=1}^{n} T_{\boldsymbol{\theta}_i} \right) \# \mu_0, \tag{1.5}$$

under specific assumptions on the optimal maps $T_{\boldsymbol{\theta}_i}$ and the reference measure μ_0 such that $\mu_{\boldsymbol{\theta}_j} = T_{\boldsymbol{\theta}_j} \# \mu_0$ for $i = 1, \ldots, n$. The validity of equation (1.5) stated in [15] is restricted to a specific class of optimal transport maps that is assumed to be admissible in the following sense (see Definition 4.2 in [15]): there exists i_0 such that $T_{\boldsymbol{\theta}_{i_0}} = I$, for each $1 \leq i \leq n$, $T_{\boldsymbol{\theta}_i}$ is a one-to-one mapping, and the composition $T_{\boldsymbol{\theta}_i} \circ T^{-1}_{\boldsymbol{\theta}_j}$ of two maps in this class remains an optimal one for all $1 \leq i, j \leq n$. The extension of the results in [15] to the population barycenter has not been considered so far. In this paper, when $\bar{T} = \mathbb{E}(T_{\boldsymbol{\theta}}) \neq I$, we do not assume that the collection of maps $(T_\theta)_{\theta \in \Theta}$ is an admissible class to prove that $\mu^* = \bar{T} \# \mu_0$, in the sense that it is

not required that $T_\theta \circ T_{\theta'}^{-1}$ is an optimal map for any $\theta, \theta' \neq \Theta$. Indeed, to prove equation (1.4), we mainly use, in this work, the assumption that $T_\theta \circ \bar{T}^{-1}$ is an optimal map for all $\theta \in \Theta$. For various deformable models of signals and images, it will be shown that such an assumption may be weaker than the notion of admissible maps introduced in [15].

Equation (1.4) is not difficult to prove in a one-dimensional setting ($d = 1$) i.e. for random measures supported on the real line. The main issue is then to extend this result to higher dimensions $d \geq 2$. To this end, we consider a dual formulation of the optimization problem (1.2) that allows a precise characterization of some properties of the population barycenter that are used to prove equation (1.4). These results are based on an adaptation of the duality arguments developed in [2] for the characterization of an empirical barycenter. Therefore, our approach is very much connected with the theory of optimal mass transport, and with the characterization of the Monge-Kantorovich problem via arguments from convex analysis and duality, see [42] for further details on this topic.

Another contribution of this paper is to discuss the usefulness of barycenters in the Wasserstein space for the statistical analysis of deformable models in signal and image processing. Statistical deformable models are widely used for the analysis of a sequence of random signals or images showing a significant amount of geometric variability in time or space. We refer to [5] for a detailed review of deformable models. In such settings, it is of fundamental interest to propose a consistent notion of averaging for signals or images sampled from such models. In this paper, we study random measures $\mu_{\boldsymbol{\theta}}$ whose associated densities $q_{\boldsymbol{\theta}}$ satisfy the following semi-parametric deformable model:

$$q_{\boldsymbol{\theta}}(x) = \left|\det\left(D\varphi_{\boldsymbol{\theta}}^{-1}\right)(x)\right| q_0\left(\varphi_{\boldsymbol{\theta}}^{-1}(x)\right) \;\; x \in \Omega, \tag{1.6}$$

where $\varphi_{\boldsymbol{\theta}} : \Omega \to \Omega$ is a random parametric diffeomorphism, $\det\left(D\varphi_{\boldsymbol{\theta}}^{-1}\right)(x)$ denotes the determinant of its Jacobian matrix at point x, and q_0 is a fixed reference density. In model (1.6), it seems natural to define the "average of $q_{\boldsymbol{\theta}}$" as the density $\bar{q}$ given by

$$\bar{q}(x) = \left|\det\left(D\bar{\varphi}^{-1}\right)(x)\right| q_0\left(\bar{\varphi}^{-1}(x)\right) \;\; x \in \Omega,$$

where $\bar{\varphi} : \Omega \to \Omega$ is defined by $\bar{\varphi}(x) = \mathbb{E}\left(\varphi_{\boldsymbol{\theta}}(x)\right) = \int_\Omega \varphi_\theta(x) g(\theta) d\theta$, $x \in \Omega$. In this paper, a novel result is to propose sufficient conditions on the random diffeomorphism $\varphi_{\boldsymbol{\theta}}$ which ensure that the measure $\bar{\mu}$ with density $\bar{q}$ corresponds to the population barycenter in the Wasserstein space of the random measure $\mu_{\boldsymbol{\theta}}$.

Finally, we also study the consistency of the empirical barycenter $\bar{\boldsymbol{\mu}}_n$ to its population counterpart μ^* as the number n of measures tends to infinity.

1.3 Related results in the literature

A similar notion (to the one in this paper) of a population barycenter and its connection to optimal transportation with infinitely many marginals have been studied in [35]. In particular, a similar class of parametric random probability measures, where the parameter set Θ is one-dimensional, is also considered in [35] for the purpose of studying the existence and uniqueness of μ^*. Some generalization of these notions for probability measures defined on a Riemannian

manifold, equipped with the Wasserstein metric, have been recently proposed in [32] and [31]. A detailed characterization of empirical barycenters, in a broader setting, in terms of existence, uniqueness and regularity, together with its link to the multi-marginal problem in optimal transport can be found in [2].

In the literature on signal and image processing, there exists various applications of the notion of an empirical barycenter in the Wasserstein space. For example, it has been successfully used for texture analysis in image processing [16, 36]. There also exists a growing interest on the development of fast algorithms for the computation of empirical barycenters with various applications in image processing [8, 17]. The theory of optimal transport for image warping has also been shown to be usefull tool, see e.g. [27, 28] and references therein. Some properties of the empirical barycenter in the 2-Wasserstein space of random measures satisfying a deformable model similar to (1.6) have also been studied in [15]. To study the registration problem of distributions, the use of semi-parametric models of densities similar to (1.6) has also been considered in [3].

The main contribution of this paper, with respect to existing results in the literature, is to show the benefits of considering the dual formulation of the (primal) problem (1.2) to characterize the population barycenter in the 2-Wasserstein space for a large class of deformable models of measures/densities. To the best of our knowledge, the characterization of a population barycenter in deformable models throughout such arguments is novel.

1.4 Organisation of the paper

The paper is then organized as follows. In Section 2, we introduce some definitions and notation for the framework of the paper, and we discuss the existence and uniqueness of the population barycenter. In Section 3, we characterize the population barycenter in the one-dimensional case, i.e. for random measures supported on $\Omega \subset \mathbb{R}$. In Section 4, we study a dual formulation of the optimization problem (1.2). In Section 5, we prove the main result of the paper, namely equation (1.4) in dimension $d \geq 2$. As an application of the methodology developed in this paper, we discuss, in Section 6, the usefulness of barycenters in the Wasserstein space for the analysis of deformable models in statistics. The consistency of the empirical barycenter is discussed in Section 7. In Section 8 , we give some perspectives on the extension of this work.

2 Existence and uniqueness of the population barycenter

2.1 Some definitions and notation

We use bold symbols $\mathbf{Y}, \boldsymbol{\mu}, \boldsymbol{\theta}, \ldots$ to denote random objects. The notation $|x|$ is used to denote the usual Euclidean norm of a vector $x \in \mathbb{R}^m$, the notation $\langle x, y \rangle$ denotes the usual inner product for $x, y \in \mathbb{R}^m$, and $\mathcal{M}_+(\Omega)$ is the set of Radon probability measures on Ω. We recall the following assumptions that are made throughout the paper.

Assumption 1. *The sets $\Omega \subset \mathbb{R}^d$ and $\Theta \subset \mathbb{R}^p$ are compact.*

Assumption 2. *The mapping* $\Phi : (\Theta \subset \mathbb{R}^p, \mathcal{B}(\mathbb{R}^p)) \to (\mathcal{M}_+(\Omega), \mathcal{B}(\mathcal{M}_+(\Omega))$ *is measurable. Moreover, it is such that, for any* $\theta \in \Theta$*, the measure* $\mu_\theta = \Phi(\theta) \in \mathcal{M}_+(\Omega)$ *admits a density with respect to the Lebesgue measure on* $\mathbb{R}^d$*.*

The squared 2-Wasserstein distance between two probability measures $\mu, \nu \in \mathcal{M}_+(\Omega)$ is

$$d^2_{W_2}(\mu,\nu) := \inf_{\gamma \in \Pi(\mu,\nu)} \left\{ \int_{\Omega\times\Omega} |x-y|^2 d\gamma(x,y) \right\},$$

where $\Pi(\mu,\nu)$ is the set of all probability measures on $\Omega \times \Omega$ having μ and ν as marginals, see e.g. [42]. We recall that $\tilde{\gamma} \in \Pi(\mu,\nu)$ is called an optimal transport plan between μ and ν if

$$d^2_{W_2}(\mu,\nu) = \int_{\Omega\times\Omega} |x-y|^2 d\tilde{\gamma}(x,y).$$

Let $T : \Omega \to \Omega$ be a measurable mapping, and let $\mu \in \mathcal{M}_+(\Omega)$. The push-forward measure $T\#\mu$ of μ through the map T is the measure defined by duality as

$$\int_\Omega f(x) d(T\#\mu)(x) = \int_\Omega f(T(x)) d\mu(x), \quad \text{for all continuous and bounded functions } f : \Omega \longrightarrow \mathbb{R}.$$

We also recall the following well known result in optimal transport (see e.g. [42] or Proposition 3.3 in [2]):

Proposition 2.1. *Let* $\mu, \nu \in \mathcal{M}_+(\Omega)$*. Then,* $\gamma \in \Pi(\mu,\nu)$ *is an optimal transport plan between* μ *and* ν *if and only if the support of* γ *is included in the set* $\partial\phi$ *that is the graph of the subdifferential of a convex and lower semi-continuous function* ϕ *satisfying*

$$\phi = \arg\min_{\psi \in \mathcal{C}} \left\{ \int_\Omega \psi(x) d\mu(x) + \int_\Omega \psi^*(x) d\nu(x) \right\},$$

where $\psi^*(x) = \sup_{y\in\Omega} \{\langle x, y\rangle - \psi(y)\}$ *is the convex conjugate of* ψ*, and* $\mathcal{C}$ *denotes the set of proper convex functions* $\psi : \Omega \to \mathbb{R}$ *that are lower semi-continuous*

If μ *admits a density with respect to the Lebesgue measure on* $\mathbb{R}^d$*, then there exists a unique optimal transport plan* $\gamma \in \Pi(\mu,\nu)$ *that is of the form* $\gamma = (id, T)\#\mu$ *where* $T = \nabla\phi$ *(the gradient of* ϕ*) is called the optimal mapping between* μ *and* ν*. The uniqueness of the transport plan holds in the sense that if* $\nabla\phi\#\mu = \nabla\psi\#\mu$*, where* $\psi : \Omega \to \mathbb{R}$ *is a lower semi-continuous convex function, then* $\nabla\phi = \nabla\psi$ *μ-almost everywhere. Moreover, one has that*

$$d^2_{W_2}(\mu,\nu) = \int_\Omega |\nabla\phi(x) - x|^2 d\mu(x).$$

2.2 About the measurability of T_θ

Let μ_0 be a fixed reference measure that is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}^d$. In the introduction, for any $\theta \in \Theta$, we have defined $T_\theta : \Omega \to \Omega$ as the optimal mapping to transport μ_0 onto μ_θ. By Proposition 2.1, such a mapping exists, and it is the μ_0-almost everywhere unique one that can be written as the gradient of a convex function ϕ_θ.

Then, thanks to Assumption 2, it follows, by Theorem 1.1 in [21], that there exists a function $(\theta, x) \mapsto T(\theta, x)$ which is measurable with respect to the σ-algebra $\mathcal{B}(\mathbb{R}^p) \otimes \mathcal{B}(\mathcal{M}_+(\Omega))$, and such that for $\mathbb{P}_\Theta$-almost everywhere $\theta \in \Theta$,

$$T(\theta, x) = T_\theta(x), \quad \text{for } \mu_0\text{-almost everywhere } x \in \Omega.$$

In particular, the mapping $(x, \theta) \mapsto T_\theta(x)$ is measurable with respect to the completion of $\mathcal{B}(\mathbb{R}^p) \otimes \mathcal{B}(\mathcal{M}_+(\Omega))$ with respect to $g(\theta)d\theta d\mu_0(x)$ (we recall the assumption that $d\mathbb{P}_\Theta(\theta) = g(\theta)d\theta$).

2.3 Existence and uniqueness of μ^*

Let us now prove the existence and uniqueness of the barycenter (i.e. the Fréchet mean) of the parametric random measures $\mu_{\boldsymbol{\theta}}$ with distribution $\mathbb{P}_g$, as defined in equation (1.1). We recall that this amounts to study the solution (if any) of the optimization problem (1.2).

Remark 2.1 (About the existence and finiteness of $J(\nu)$)**.** *Let $\nu \in \mathcal{M}_+(\Omega)$. The integral defining $J(\nu)$ will be defined as soon as $\theta \mapsto d^2_{W_2}(\nu, \mu_\theta)g(\theta)$ is a measurable application. The measurability of this mapping follows from Assumption 2. Moreover, since Ω is compact by Assumption 1, it follows that, for any $\theta \in \Theta$, $d^2_{W_2}(\nu, \mu_\theta) \leq 4\delta^2(\Omega)$, where $\delta^2(\Omega) = \sup_{x\in\Omega}\{|x|^2\} < +\infty$. Therefore, one has that $J(\nu) = \frac{1}{2}\int_\Theta d^2_{W_2}(\nu, \mu_\theta)g(\theta)d\theta \leq 2\delta^2(\Omega) < +\infty$, for any $\nu \in \mathcal{M}_+(\Omega)$.*

As shown below, using standard arguments, the existence and the uniqueness of μ^* are not difficult to prove. To this end, a key property of the functional J defined in (1.2) is the following:

Lemma 2.1. *Suppose that Assumption 2 holds. Then, the functional $J : \mathcal{M}_+(\Omega) \to \mathbb{R}$ is strictly convex in the sense that*

$$J(\lambda\mu + (1-\lambda)\nu) < \lambda J(\mu) + (1-\lambda)J(\nu), \text{ for any } \lambda \in]0,1[\text{ and } \mu, \nu \in \mathcal{M}_+(\Omega) \text{ with } \mu \neq \nu. \quad (2.1)$$

Proof. Inequality (2.1) follows immediately from the assumption that, for any $\theta \in \Theta$, the measure μ_θ admits a density with respect to the Lebesgue measure on $\mathbb{R}^d$, and from the use of Theorem 2.9 in [6] (for similar results to those in [6] on the strict convexity, one can read Lemma 3.2.1 in [35]). □

Hence, thanks to the strict convexity of J, if a barycenter μ^* exists, then it is necessarily unique. The existence of μ^* is then proved in the next proposition.

Proposition 2.2. *Under Assumption 1 and Assumption 2, the optimization problem (1.2) admits a unique minimizer.*

Proof. Let ν^n be a minimizing sequence of the optimization problem (1.2). Let us first show that the sequence $\int_\Omega |x|^2 d\nu^n(x)$ is uniformly bounded. Thanks to Remark 2.1, there exists a constant $C > 0$ such that $\int_\Theta \frac{1}{2}d^2_{W_2}(\mu_\theta, \nu^n)g(\theta)d\theta \leq C$, for all $n \geq 1$. Since g is a probability density function on Θ with respect to the Lebesgue measure, it follows that $\Theta' := \{\theta, g(\theta) > 0\}$ is a non negligible set (for the Lebesgue's measure). Since $\int_{\Theta'} \frac{1}{2}d^2_{W_2}(\mu_\theta, \nu^n)g(\theta)d\theta \leq C$, one obtains that there exists $\theta^* \in \Theta'$, such that $g(\theta^*) \neq 0$ and

$$\frac{1}{2}d^2_{W_2}(\mu_{\theta^*}, \nu^n)g(\theta^*) \leq C' \quad (2.2)$$

where $C' = \frac{C}{\int_{\Theta'} d\theta}$. Then, thanks to the Kantorovich duality formula (see e.g. [42], or Lemma 2.1 in [2]) , it follows that

$$\frac{1}{2} d^2_{W_2}(\mu_{\theta^*}, \nu^n) g(\theta^*) \geq \int_\Omega |x|^2 d\nu^n(x) + \int_\Omega C_{g(\theta^*)}(x) d\mu_{\theta^*}(x),$$

where $C_{g(\theta^*)}(x) = \inf_{y \in \Omega} \left\{ \frac{g(\theta^*)}{2} |x-y|^2 - |y|^2 \right\}$. Note that by Assumption 1, Ω is a compact set, and therefore the function $x \mapsto |C_{g(\theta^*)}(x)|$ is bounded on Ω. Hence, combining the above inequality with (2.2), one finally obtains that

$$\int_\Omega |x|^2 d\nu^n(x) \leq C' - \int_\Omega C_{g(\theta^*)}(x) d\mu_{\theta^*}(x), \text{ for all } n \geq 1,$$

which shows that $\int_\Omega |x|^2 d\nu^n(x)$ is a uniformly bounded sequence.

Hence, by Chebyshev's inequality, the sequence ν_n is tight and by Prokhorov's Theorem there exists a (non relabeled) subsequence that weakly converges to some $\mu^* \in \mathcal{M}_+(\Omega)$. Therefore, $\frac{1}{2} d^2_{W_2}(\mu_\theta, \mu^*) \leq \liminf_{n \to +\infty} \frac{1}{2} d^2_{W_2}(\mu_\theta, \nu^n)$, and thus, by Fatou's Lemma

$$\int_\Theta \frac{1}{2} d^2_{W_2}(\mu_\theta, \mu^*) g(\theta) d\theta \leq \int_\Theta \liminf_{n \to +\infty} \frac{1}{2} d^2_{W_2}(\mu_\theta, \nu^n) g(\theta) d\theta \leq \liminf_{n \to +\infty} \int_\Theta \frac{1}{2} d^2_{W_2}(\mu_\theta, \nu^n) g(\theta) d\theta.$$

Therefore, $J(\mu^*) = \inf_{\nu \in \mathcal{M}_+(\Omega)} \frac{1}{2} \int_\Theta d^2_{W_2}(\nu, \mu_\theta) g(\theta) d\theta$, which proves that the optimization problem (1.2) admits a minimizer.

By the strict convexity of the functional J (as stated in Lemma 2.1), it follows that the barycenter of $\mu_{\boldsymbol{\theta}}$ is necessarily unique. □

3 Barycenter for measures supported on the real line

In this section, we study some properties of the population barycenter μ^* of random measures supported on the real line i.e. we consider the case $d = 1$ where Ω is a compact subset of $\mathbb{R}$. In this setting, our characterization of μ^* will follow from the well known fact that if μ and ν are measures belonging to $\mathcal{M}_+(\Omega)$ then

$$d^2_{W_2}(\nu, \mu) = \int_0^1 \left| F^{-1}_\nu(x) - F^{-1}_\mu(x) \right|^2 dx, \tag{3.1}$$

where F^{-1}_ν (resp. F^{-1}_μ) is the quantile function of ν (resp. μ). This explicit expression for the Wasserstein distance allows a simple characterization of the barycenter of random measures. In particular, we prove that equation (1.4) always holds for $d = 1$. This result means that, in dimension 1, computing a barycenter in the Wasserstein space amounts to take the expectation (in the usual sense) of the optimal mapping to transport a fixed (non-random) reference measure μ_0 onto $\mu_{\boldsymbol{\theta}}$.

Theorem 3.1. *Let μ_0 be any fixed measure in $\mathcal{M}_+(\Omega)$ that is absolutely continuous with respect to the Lebesgue measure. Suppose that Assumption 1 and Assumption 2 hold. Let $\mu_{\boldsymbol{\theta}} = \Phi(\boldsymbol{\theta})$*

be a random measure where $\boldsymbol{\theta}$ *is a random vector in* Θ *with density* g*. Let* $T_{\boldsymbol{\theta}}$ *be the random optimal mapping between* μ_0 *and* $\mu_{\boldsymbol{\theta}}$ *given by* $T_{\boldsymbol{\theta}}(x) = F^{-1}_{\mu_{\boldsymbol{\theta}}}(F_{\mu_0}(x))$*,* $x \in \Omega$*, where* $F^{-1}_{\mu_{\boldsymbol{\theta}}}$ *is the quantile function of* $\mu_{\boldsymbol{\theta}}$*, and* F_{μ_0} *is the cumulative distribution function of* μ_0*.*

Then, the barycenter of $\mu_{\boldsymbol{\theta}}$ *exists, it is unique, and it satisfies the equation*

$$\mu^* = \bar{T}\#\mu_0, \tag{3.2}$$

where $\bar{T} : \Omega \to \Omega$ *denotes the optimal mapping between* μ_0 *and* μ^* *that is defined by*

$$\bar{T}(x) = \mathbb{E}\left(T_{\boldsymbol{\theta}}(x)\right) = \int_\Theta T_\theta(x) g(\theta) d\theta, \text{ for all } x \in \Omega.$$

Furthermore, the quantile function of μ^* *is*

$$F^{-1}_{\mu^*}(y) = \mathbb{E}\left(F^{-1}_{\mu_{\boldsymbol{\theta}}}(y)\right) = \int_\Theta F^{-1}_{\mu_\theta}(y) g(\theta) d\theta,$$

for $y \in [0,1]$*. Thus, the barycenter* μ^* *does not depend on the choice of* μ_0*, and one has that*

$$\inf_{\nu \in \mathcal{M}_+(\Omega)} J(\nu) = \frac{1}{2}\int_\Omega \mathbb{E}\left(|\bar{T}_{\boldsymbol{\theta}}(x) - x|^2\right) d\mu^*(x) = \frac{1}{2}\int_\Omega \int_\Theta |\bar{T}_\theta(x) - x|^2 g(\theta) d\theta d\mu^*(x), \tag{3.3}$$

where $\bar{T}_{\boldsymbol{\theta}} = T_{\boldsymbol{\theta}} \circ \bar{T}^{-1}$*.*

Proof. Let $\nu \in \mathcal{M}_+(\Omega)$ then

$$J(\nu) = \int_\Theta \frac{1}{2} d^2_{W_2}(\nu, \mu_\theta) g(\theta) d\theta = \frac{1}{2}\int_\Theta \int_0^1 \left|F^{-1}_\nu(y) - F^{-1}_{\mu_\theta}(y)\right|^2 dy g(\theta) d\theta.$$

In the proof, we will repeatedly use Fubini's Theorem to interchange the order of integration in the right-hand size of the above equation. To be valid, Fubini's Theorem requires that the application $(y,\theta) \mapsto \left|F^{-1}_\nu(y) - F^{-1}_{\mu_\theta}(y)\right|^2 g(\theta)$ is measurable. This application will be measurable as soon as $(y,\theta) \mapsto F^{-1}_{\mu_\theta}(y)$ is measurable. Since, by definition, $F^{-1}_{\mu_\theta}(y) = T_\theta(F^{-1}_{\mu_0}(y))$ for any $y \in [0,1]$, the measurability of $(y,\theta) \mapsto F^{-1}_{\mu_\theta}(y)$ is ensured by the continuity of $y \mapsto F^{-1}_{\mu_0}(y)$ and the measurability of the mapping $(x,\theta) \mapsto T_\theta(x)$ which has been stated in Section 2.2.

Let us now consider the function $\mathbb{E}\left(F^{-1}_{\mu_{\boldsymbol{\theta}}}\right) : [0,1] \to \Omega$ defined by

$$\mathbb{E}\left(F^{-1}_{\mu_{\boldsymbol{\theta}}}\right)(y) := \mathbb{E}\left(F^{-1}_{\mu_{\boldsymbol{\theta}}}(y)\right) = \int_\Theta F^{-1}_{\mu_\theta}(y) g(\theta) d\theta < +\infty$$

for any $y \in [0,1]$. We will now prove that $\mathbb{E}\left(F^{-1}_{\mu_{\boldsymbol{\theta}}}\right)$ is a quantile function. To this end, let $\delta^2(\Omega) = \sup_{x\in\Omega}\{|x|^2\}$ that is finite by Assumption 1 (compactness of Ω). Then, by Assumption 2, the measure μ_θ admits a density with respect to the Lebesgue measure, and thus the function $y \mapsto F^{-1}_{\mu_\theta}(y)$ is continuous on $[0,1]$, for any $\theta \in \Theta$. Hence, since $|F^{-1}_{\mu_\theta}(y)| \leq \delta(\Omega)$ for any $(\theta, y) \in \Theta \times [0,1]$ it follows, by Lebesgue's dominated convergence theorem, that $y \mapsto \mathbb{E}\left(F^{-1}_{\mu_{\boldsymbol{\theta}}}\right)(y)$ is a continuous function on $[0,1]$. Since $y \mapsto F^{-1}_{\mu_\theta}(y)$ is increasing for any $\theta \in \Theta$, it is also clear that

$y \mapsto \mathbb{E}\left(F^{-1}_{\mu_{\boldsymbol{\theta}}}\right)(y)$ is an increasing function. Hence, thanks to the property that any continuous and increasing function from $[0,1]$ to Ω is the quantile of some probability measure belonging to $\mathcal{M}_+(\Omega)$ (see e.g. [20]), one obtains that $\mathbb{E}\left(F^{-1}_{\mu_{\boldsymbol{\theta}}}\right)$ is a quantile function.

Now, it is clear that $\mathbb{E}\left(|F^{-1}_{\mu_{\boldsymbol{\theta}}}(y)|^2\right) \leq \delta^2(\Omega) < +\infty$ for any $y \in [0,1]$. Hence, applying Fubini's Theorem, and the fact that $\mathbb{E}\,|a-X|^2 \geq \mathbb{E}\,|\mathbb{E}(X)-X|^2$ for any squared integrable real random variable X and real number a, we obtain that

$$\begin{aligned}
\int_\Theta d^2_{W_2}(\nu,\mu_\theta)g(\theta)d\theta &= \int_0^1\int_\Theta \left|F^{-1}_\nu(y)-F^{-1}_{\mu_\theta}(y)\right|^2 g(\theta)d\theta dy = \int_0^1 \mathbb{E}\left|F^{-1}_\nu(y)-F^{-1}_{\mu_{\boldsymbol{\theta}}}(y)\right|^2 dy \\
&\geq \int_0^1 \mathbb{E}\left|\mathbb{E}\left(F^{-1}_{\mu_{\boldsymbol{\theta}}}(y)\right)-F^{-1}_{\mu_{\boldsymbol{\theta}}}(y)\right|^2 dy \\
&= \int_0^1\int_\Theta \left|\mathbb{E}\left(F^{-1}_{\mu_{\boldsymbol{\theta}}}(y)\right)-F^{-1}_{\mu_\theta}(y)\right|^2 g(\theta)d\theta dy \\
&= \int_\Theta d^2_{W_2}(\mu^*,\mu_\theta)g(\theta)d\theta, \qquad (3.4)
\end{aligned}$$

where μ^* is the measure in $\mathcal{M}_+(\Omega)$ with quantile function given by $F^{-1}_{\mu^*} = \mathbb{E}\left(F^{-1}_{\mu_{\boldsymbol{\theta}}}\right)$. The above inequality shows that $J(\nu) \geq J(\mu^*)$ for any $\nu \in \mathcal{M}_+(\Omega)$. Therefore, μ^* is a barycenter of the random measure $\mu_{\boldsymbol{\theta}}$, and the unicity of μ^* follows from the strict convexity of the functional J as stated in Lemma 2.1. Finally, let μ_0 be any fixed measure in $\mathcal{M}_+(\Omega)$ that is absolutely continuous with respect to the Lebesgue measure. Hence, one has that $F_{\mu_0}\circ F^{-1}_{\mu_0}(y) = y$ for any $y \in [0,1]$. Therefore, equation (3.2) follows from the equalities

$$F^{-1}_{\mu^*} = \mathbb{E}\left(F^{-1}_{\mu_{\boldsymbol{\theta}}}\right) = \mathbb{E}\left(F^{-1}_{\mu_{\boldsymbol{\theta}}}\circ F_{\mu_0}\right)\circ F^{-1}_{\mu_0} = \mathbb{E}\left(T_{\boldsymbol{\theta}}\right)\circ F^{-1}_{\mu_0} = \bar{T}\circ F^{-1}_{\mu_0},$$

where $\bar{T} = \mathbb{E}\left(T_{\boldsymbol{\theta}}\right) = F^{-1}_{\mu^*}\circ F_{\mu_0}$. Note that it is clear that $\bar{T}:\Omega\to\Omega$ is an increasing and continuous function, and thus it is the optimal mapping between μ_0 and μ^* by Proposition 2.1. Finally, by equation (3.4) and Fubini's Theorem, one has that

$$\begin{aligned}
\int_\Theta d^2_{W_2}(\mu^*,\mu_\theta)g(\theta)d\theta &= \int_0^1 \mathbb{E}\left|F^{-1}_{\mu^*}(y)-F^{-1}_{\mu_{\boldsymbol{\theta}}}(y)\right|^2 dy = \mathbb{E}\left(\int_0^1 \left|F^{-1}_{\mu^*}(y)-F^{-1}_{\mu_{\boldsymbol{\theta}}}(y)\right|^2 dy\right) \\
&= \mathbb{E}\left(\int_\Omega \left|F^{-1}_{\mu_{\boldsymbol{\theta}}}\circ F_{\mu^*}(x)-x\right|^2 d\mu^*(x)\right) \\
&= \mathbb{E}\left(\int_\Omega \left|F^{-1}_{\mu_{\boldsymbol{\theta}}}\circ F_{\mu_0}\circ F^{-1}_{\mu_0}\circ F_{\mu^*}(x)-x\right|^2 d\mu^*(x)\right) \\
&= \mathbb{E}\left(\int_\Omega \left|T_{\boldsymbol{\theta}}\circ \bar{T}^{-1}(x)-x\right|^2 d\mu^*(x)\right)
\end{aligned}$$

where the last equality follows from the fact that $T_{\boldsymbol{\theta}} = F^{-1}_{\mu_{\boldsymbol{\theta}}}\circ F_{\mu_0}$ and $\bar{T}^{-1} = F^{-1}_{\mu_0}\circ F_{\mu^*}$. Hence, this proves equation (3.3), and it completes the proof.

□

To illustrate Theorem 3.1, we consider a simple construction of random probability measures in the case where Ω is a compact interval of $\mathbb{R}$. Let $\bar{\mu} \in \mathcal{M}_+^2(\Omega)$ admitting the density $\bar{f}$ with respect to the Lebesgue measure on $\mathbb{R}$, and cumulative distribution function (cdf) $\bar{F}$. We assume that the density $\bar{f}$ is continuous on Ω, and that it is compactly supported in a sub-interval Ω_0 of Ω. Let $\boldsymbol{\theta} = (\mathbf{a}, \mathbf{b}) \in]0, +\infty[\times\mathbb{R}$ be a two dimensional random vector with density g, such that $\mathbf{a}x + \mathbf{b} \in \Omega$ for any $x \in \Omega_0$. We denote by $\mu_{\boldsymbol{\theta}}$ the random probability measure admitting the density

$$f_{\boldsymbol{\theta}}(x) = \frac{1}{\mathbf{a}} \bar{f}\left(\frac{x - \mathbf{b}}{\mathbf{a}}\right), \ x \in \Omega,$$

where we have extended $\bar{f}$ outside Ω by letting $\bar{f}(u) = 0$ for $u \notin \Omega$. Thanks to our assumptions, the density $f_{\boldsymbol{\theta}}$ is compactly supported in a sub-interval of Ω. Moreover, the cdf and quantile function of $\mu_{\boldsymbol{\theta}}$ are given by

$$F_{\mu_{\boldsymbol{\theta}}}(x) = \bar{F}\left(\frac{x - \mathbf{b}}{\mathbf{a}}\right), \ x \in \Omega, \quad \text{and} \quad F^{-1}_{\mu_{\boldsymbol{\theta}}}(y) = \mathbf{a}\bar{F}^{-1}(y) + \mathbf{b}, \ y \in [0, 1].$$

By Theorem 3.1, it follows that the barycenter of $\mu_{\boldsymbol{\theta}}$ is the probability measure μ^* whose quantile function is given by

$$F^{-1}_{\mu^*}(y) = \mathbb{E}(\mathbf{a})\bar{F}^{-1}(y) + \mathbb{E}(\mathbf{b}), \ y \in [0, 1].$$

Therefore, μ^* admits the density

$$f^*(x) = \frac{1}{\mathbb{E}(\mathbf{a})} \bar{f}\left(\frac{x - \mathbb{E}(\mathbf{b})}{\mathbb{E}(\mathbf{a})}\right), x \in \Omega,$$

with respect to the Lebesgue measure on $\mathbb{R}$. Moreover, if μ_0 is any fixed measure in $\mathcal{M}_+(\Omega)$, that is absolutely continuous with respect to the Lebesgue measure, then

$$\mu^* = T_0 \# \mu_0, \quad \text{where} \quad T_0(x) = \mathbb{E}(\mathbf{a})\bar{F}^{-1}(F_{\mu_0}(x)) + \mathbb{E}(\mathbf{b}), \ x \in \Omega.$$

Now, we remark that extending Theorem 3.1 to dimension $d \geq 2$ is not straightforward. Indeed, the two key ingredients in the proof of Theorem 3.1 are the use of the well-known characterization (3.1) of the Wasserstein distance in dimension $d = 1$ via the quantile functions, and the fact that, in dimension $d = 1$, the composition of two optimal maps (which are increasing functions) remains an optimal one (thanks to Proposition 2.1). However, the property (3.1) which explicitly relates the Wasserstein distance $d_{W_2}(\nu, \mu_\theta)$ to the marginal distributions of ν and μ_θ is not valid in higher dimensions. Moreover, the composition of two optimal maps is not necessarily an optimal one in dimension $d \geq 2$. Nevertheless, we show in Section 5 that analogs of Theorem 3.1 can still be obtained in dimension $d \geq 2$.

4 Dual formulation

In this section, we introduce a dual formulation of problem (1.2) that is inspired by the one proposed in [2] to study the properties of empirical barycenters. This dual formulation is then

the key property to state the main result of this paper given in Section 5. Let us recall the optimization problem (1.2) as

$$(\mathcal{P}) \quad J_{\mathcal{P}} := \inf_{\nu \in \mathcal{M}_+(\Omega)} J(\nu), \text{ where } J(\nu) = \frac{1}{2} \int_\Theta d^2_{W_2}(\nu, \mu_\theta) g(\theta) d\theta. \tag{4.1}$$

Then, let us introduce some definitions. Let $X = C(\Omega, \mathbb{R})$ be the space of continuous functions $f : \Omega \to \mathbb{R}$ equipped with the supremum norm

$$\|f\|_X = \sup_{x \in \Omega} \{|f(x)|\}.$$

We also denote by $X' = \mathcal{M}(\Omega)$ the topological dual of X. The notation $f^\Theta = (f_\theta)_{\theta \in \Theta} \in L^1(\Theta, X)$ will denote any mapping

$$\left\{ \begin{array}{rccc} f^\Theta : & \Theta & \to & X \\ & \theta & \mapsto & f_\theta \end{array} \right.$$

such that for any $x \in \Omega$

$$\int_\Theta |f_\theta(x)| d\theta < +\infty.$$

Then, following the terminology in [2], we introduce the dual optimization problem

$$(\mathcal{P}^*) \qquad J_{\mathcal{P}^*} := \sup \left\{ \int_\Theta \int_\Omega S_{g(\theta)} f_\theta(x) d\mu_\theta(x) d\theta; \ f^\Theta \in L^1(\Theta, X) \text{ such that } \int_\Theta f_\theta(x) d\theta = 0, \ \forall x \in \Omega \right\}, \tag{4.2}$$

where

$$S_{g(\theta)} f(x) := \inf_{y \in \Omega} \left\{ \frac{g(\theta)}{2} |x - y|^2 - f(y) \right\}, \forall x \in \Omega \ \text{ and } \ f \in X.$$

Let us also define

$$H_{g(\theta)}(f) := - \int_\Omega S_{g(\theta)} f(x) d\mu_\theta(x),$$

and the Legendre-Fenchel transform of $H_{g(\theta)}$ for $\nu \in X'$ as

$$H^*_{g(\theta)}(\nu) := \sup_{f \in X} \left\{ \int_\Omega f(x) d\nu(x) - H_{g(\theta)}(f) \right\} = \sup_{f \in X} \left\{ \int_\Omega f(x) d\nu(x) + \int_\Omega S_{g(\theta)} f(x) d\mu_\theta(x) \right\}.$$

In what follows, we show that the problems $(\mathcal{P})$ and $(\mathcal{P}^*)$ are dual to eachother in the sense that the minimal value $J_{\mathcal{P}}$ in problem $(\mathcal{P})$ is equal to the supremum $J_{\mathcal{P}^*}$ in problem $(\mathcal{P}^*)$. This duality is the key tool for the proof of Theorem 5.1.

Proposition 4.1. *Suppose that Assumption 1 and Assumption 2 are satisfied. Then,*

$$J_{\mathcal{P}} = J_{\mathcal{P}^*}.$$

Proof. 1. Let us first prove that $J_{\mathcal{P}} \geq J_{\mathcal{P}^*}$.
By definition for any $f^\Theta \in L^1(\Theta, X)$ such that $\forall x \in \Omega,\ \int_\Theta f_\theta(x)d\theta = 0$, and for all $y \in \Omega$ we have

$$S_{g(\theta)} f_\theta(x) + f_\theta(y) \leq \frac{g(\theta)}{2}|x-y|^2.$$

Let $\nu \in \mathcal{M}_+(\Omega)$ and $\gamma_\theta \in \Pi(\mu_\theta, \nu)$ be an optimal transport plan between μ_θ and ν. By integrating the above inequality with respect to γ_θ we obtain

$$\int_\Omega S_{g(\theta)} f_\theta(x) d\mu_\theta(x) + \int_\Omega f_\theta(y) d\nu(y) \leq \int_{\Omega\times\Omega} \frac{g(\theta)}{2}|x-y|^2 d\gamma_\theta(x,y) = \frac{g(\theta)}{2} d^2_{W_2}(\mu_\theta, \nu).$$

Integrating now with respect to $d\theta$ and using Fubini's Theorem we get

$$\int_\Theta \int_\Omega S_{g(\theta)} f_\theta(x) d\mu_\theta(x) d\theta \leq \int_\Theta \frac{g(\theta)}{2} d^2_{W_2}(\mu_\theta, \nu) d\theta.$$

Therefore we deduce that $J_{\mathcal{P}} \geq J_{\mathcal{P}^*}$.

2. Let us now prove the converse inequalities $J_{\mathcal{P}} \leq J_{\mathcal{P}^*}$.
Thanks to the Kantorovich duality formula (see e.g. [42], or Lemma 2.1 in [2]) we have that $H^*_{g(\theta)}(\nu) = \frac{1}{2} d^2_{W_2}(\mu_\theta, \nu) g(\theta)$ for any $\nu \in \mathcal{M}_+(\Omega)$. Therefore, it follows that

$$J_P = \inf\left\{ \int_\Theta H^*_{g(\theta)}(\nu) d\theta,\ \nu \in X' \right\} = -\left(\int_\Theta H^*_{g(\theta)} d\theta \right)^* (0). \tag{4.3}$$

Define the inf-convolution of $\left(H_{g(\theta)}\right)_{\theta\in\Theta}$ by

$$H(f) := \inf\left\{ \int_\Theta H_{g(\theta)}(f_\theta) d\theta;\ f^\Theta \in L^1(\Theta, X), \int_\Theta f_\theta(x) d\theta = f(x), \forall x \in \Omega \right\}, \quad \forall f \in X.$$

We have in the other hand that

$$J_{\mathcal{P}^*} = -H(0).$$

Using Theorem 1.6 in [33], one has that for any $\nu \in \mathcal{M}_+(\Omega)$

$$H^*(\nu) = \int_\Theta H^*_{g(\theta)}(\nu) d\theta.$$

Then, thanks to (4.3), it follows that

$$J_P = -H^{**}(0) \geq -H(0) = J_{\mathcal{P}^*}.$$

Let us now prove that $H^{**}(0) = H(0)$. Since H is convex it is sufficient to show that H is continuous at 0 for the supremum norm of the space X (see e.g. Proposition 4.1 in [19]). For this purpose, let $f^\Theta \in L^1(\Theta, X)$ and remark that it follows from the definition of $H_{g(\theta)}$ that

$$\begin{aligned} H_{g(\theta)}(f_\theta) &= \int_\Omega \sup_{y\in\Omega} \left\{ f_\theta(y) - \frac{g(\theta)}{2}|x-y|^2 \right\} d\mu_\theta(x) \\ &\geq f_\theta(0) - \frac{g(\theta)}{2} \int_\Omega |x|^2 d\mu_\theta(x), \end{aligned}$$

which implies that

$$H(f) \geq f(0) - \int_\Theta \frac{g(\theta)}{2} \int_\Omega |x|^2 d\mu_\theta(x) d\theta > -\infty, \ \forall f \in X.$$

Let $f \in X$ such that $\|f\|_X \leq 1/4$ and choose $f^\Theta \in L^1(\Theta, X)$ defined by $f_\theta(x) = f(x)g(\theta)$ for all $\theta \in \Theta$ and $x \in \Omega$. It follows that

$$\begin{aligned} H(f) &\leq \int_\Theta H_{g(\theta)}(f(\cdot)g(\theta))d\theta \leq \int_\Theta \int_\Omega \sup_{y\in\Omega} \left\{ \frac{g(\theta)}{4} - \frac{g(\theta)}{2}|x-y|^2 \right\} d\mu_\theta(x) d\theta \\ &\leq \int_\Theta \int_\Omega \frac{g(\theta)}{4} d\mu_\theta(x) d\theta = \frac{1}{4}. \end{aligned}$$

Hence, the convex function H never takes the value $-\infty$ and is bounded from above in a neighborhood of 0 in X. Therefore, by standard results in convex analysis (see e.g. Lemma 2.1 in [19]), H is continuous at 0, and therefore $H^{**}(0) = H(0)$ which completes the proof. □

5 An explicit characterization of the population barycenter

In this section, we extend the results of Theorem 3.1 to dimension $d \geq 2$. Let $\mu_{\boldsymbol{\theta}} \in \mathcal{M}_+(\Omega)$ denote the parametric random measure with distribution $\mathbb{P}_g$, as defined in equation (1.1). Let μ_0 be a fixed (reference) measure in $\mathcal{M}_+(\Omega)$ admitting a density with respect to the Lebesgue measure on $\mathbb{R}^d$. Then, by Proposition 2.1, there exists, for any $\theta \in \Theta$, a unique optimal mapping $T_\theta : \Omega \to \Omega$ such that $\mu_\theta = T_\theta \# \mu_0$, where $T_\theta = \nabla\phi_\theta$ μ_0-almost everywhere, and $\phi_\theta : \Omega \to \mathbb{R}$ is a lower semi-continuous convex (l.s.c) function.

In Theorem 5.1 below, we give sufficient conditions on the expectation of $T_{\boldsymbol{\theta}}$ which imply that the barycenter of $\mu_{\boldsymbol{\theta}}$ is given by $\mu^* = \mathbb{E}\left(T_{\boldsymbol{\theta}}\right) \# \mu_0$. This result means that computing a barycenter in the Wasserstein space amounts to take the expectation (in the usual sense) of the optimal mapping $T_{\boldsymbol{\theta}}$ to transport μ_0 onto $\mu_{\boldsymbol{\theta}}$. The proof of this result relies on the use of a dual formulation of the optimization problem (1.2) that is stated in equation (4.2), and we refer to Section 4 for further details.

Before stating the main result of this section, we introduce, for any $\theta \in \Theta$, the notation

$$\bar{T}_\theta = T_\theta \circ \bar{T}^{-1}, \tag{5.1}$$

where $\bar{T} : \Omega \to \Omega$ is the mapping defined by $\overline{T}(x) = \mathbb{E}\left(T_{\boldsymbol{\theta}}(x)\right) = \int_\Theta T_\theta(x) g(\theta) d\theta, \ x \in \Omega$. Note that equation (5.1) is only valid if $\bar{T}^{-1}$ is well defined. Sufficient conditions to ensure the existence of $\bar{T}$ as a one-to-one mapping from Ω to Ω are given in the following theorem which contains the main results of this paper.

Theorem 5.1. *Let $\boldsymbol{\theta} \in \mathbb{R}^p$ be a random vector with a density $g : \Theta \to \mathbb{R}$ such that $g(\theta) > 0$ for all $\theta \in \Theta$. Let $\mu_{\boldsymbol{\theta}} = \Phi(\boldsymbol{\theta})$ be a parametric random measure with distribution $\mathbb{P}_g$. Let μ_0 be a fixed measure in $\mathcal{M}_+(\Omega)$ admitting a density with respect to the Lebesgue measure on $\mathbb{R}^d$. Suppose that Assumption 1 and Assumption 2 hold.*

1. *If for any $\theta \in \Theta$ the following asumption holds*

$$(i) \qquad T_\theta \text{ is a } C^1 \text{ diffeomorphism of } \Omega, \tag{5.2}$$

Then, $\bar{T}$ is a measurable mapping and it is a C^1 diffeomorphism of Ω.

2. *In addition, If for any $\theta \in \Theta$ the following asumption holds*

$$(ii) \qquad \bar{T}_\theta = \nabla \bar{\phi}_\theta \text{ where } \bar{\phi}_\theta : \Omega \to \mathbb{R} \text{ is a l.s.c. convex function,} \tag{5.3}$$

such that for any $x \in \Omega$, the function $\theta \mapsto \bar{\phi}_\theta(x)$ is integrable with respect to $\mathbb{P}_\Theta$ and satisfies the normalization condition

$$\int_\Theta \bar{\phi}_\theta(x) g(\theta) d\theta = \frac{1}{2}|x|^2 \text{ for all } x \in \Omega. \tag{5.4}$$

Then the population barycenter is the measure $\mu^* \in \mathcal{M}_+(\Omega)$ given by

$$\mu^* = \overline{T} \# \mu_0, \tag{5.5}$$

and the optimization problem (1.2) satisfies

$$\inf_{\nu \in \mathcal{M}_+(\Omega)} J(\nu) = \frac{1}{2} \int_\Theta d^2_{W_2}(\mu^*, \mu_\theta) g(\theta) d\theta = \frac{1}{2} \int_\Omega \mathbb{E}\left(|\bar{T}_{\boldsymbol{\theta}}(x) - x|^2\right) d\mu^*(x). \tag{5.6}$$

Proof. Under the assumptions of Theorem 5.1, it follows from Proposition 2.2 that the barycenter μ^* exists and is unique.

Let us first prove that Condition (5.2) implies that $\bar{T}_\theta = T_\theta \circ \bar{T}^{-1}$ is a C^1 diffeomorphism. By our remarks in Section 2.2, one has that $(x, \theta) \mapsto T_\theta(x)$ is a mesurable mapping with respect to the completion of $\mathcal{B}(\mathbb{R}^p) \otimes \mathcal{B}(\mathcal{M}_+(\Omega))$ with respect to $g(\theta) d\theta d\mu_0(x)$. Therefore, $x \mapsto \bar{T}(x)$ is also a mesurable mapping. Using Assumption 1 (compactness of Ω), Condition (5.2), and Lebesgue's dominated convergence theorem, it can be checked that $\bar{T}$ is a C^1 diffeomorphism of Ω, which implies that $\bar{T}_\theta = T_\theta \circ \bar{T}^{-1}$ is also a C^1 diffeomorphism of Ω for any $\theta \in \Theta$.

The rest of the proof relies on the dual formulation (4.2) of the optimization problem (1.2), and we refer to Section 4 for further details and notation. To prove the results stated in Theorem 5.1, we will use the dual characterization of the barycenter μ^* that is stated in Proposition 4.1. For this purpose, we need to find a maximizer $f^\Theta = (f_\theta)_{\theta \in \Theta} \in L^1(\Theta, X)$ of the dual problem $(\mathcal{P}^*)$, see equation (4.2). In the proof, we repeatedly use the fact that $\mu_\theta = \bar{T}_\theta \# \bar{\mu}$ where, by definition, $\bar{\mu} = \bar{T} \# \mu_0$, and the property that $\bar{T}_\theta = T_\theta \circ \bar{T}^{-1}$ is a C^1 diffeomorphism.

a) Let us first compute an upper bound of $J_{\mathcal{P}^*}$. Let $f^\Theta \in L^1(\Theta, X)$ be such that $\int_\Theta f_\theta(x) d\theta = 0$ for all $x \in \Omega$. By definition of $S_{g(\theta)} f_\theta(x)$ one has that

$$S_{g(\theta)} f_\theta(x) \leq \frac{g(\theta)}{2}|x - y|^2 - f_\theta(y) \tag{5.7}$$

for any $y \in \Omega$. By using inequality (5.7) with $y = \bar{T}_\theta^{-1}(x)$ for $x \in \Omega$, one obtains that

$$\begin{aligned}\int_\Theta \int_\Omega S_{g(\theta)} f_\theta(x) d\mu_\theta(x) d\theta &\leq \int_\Theta \int_\Omega \left(\frac{g(\theta)}{2} |x - \bar{T}_\theta^{-1}(x)|^2 - f_\theta\left(\bar{T}_\theta^{-1}(x)\right) \right) d\mu_\theta(x) d\theta \\ &= \int_\Theta \int_\Omega \left(\frac{g(\theta)}{2} |\bar{T}_\theta(u) - u|^2 - f_\theta(u) \right) d\bar{\mu}(u) d\theta \\ &= \int_\Theta \int_\Omega \left(\frac{g(\theta)}{2} |\bar{T}_\theta(u) - u|^2 \right) d\bar{\mu}(u) d\theta\end{aligned}$$

Note that to obtain the second inequality above, we have used the change of variable $u = \bar{T}_\theta^{-1}(x)$, while the third inequality has been obtained using the fact that $\int_\Theta f_\theta(u)\, d\theta = 0$ for any $u \in \Omega$ combined with Fubini's theorem. Thanks to Condition 5.3, $\bar{T}_{\boldsymbol{\theta}}$ is the gradient of a convex function, and it is such that $\mu_\theta = \bar{T}_\theta \# \bar{\mu}$. Hence, by Proposition 2.1, one obtains that $\int_\Omega |\bar{T}_\theta(u) - u|^2 d\bar{\mu}(u) = d^2_{W_2}(\bar{\mu}, \mu_\theta)$ which implies that

$$\begin{aligned}J(\bar{\mu}) &= \int_\Theta \frac{1}{2} d^2_{W_2}(\bar{\mu}, \mu_\theta) g(\theta) d\theta, \\ &= \int_\Theta \int_\Omega \left(\frac{g(\theta)}{2} |\bar{T}_\theta(u) - u|^2 \right) d\bar{\mu}(u) d\theta = \frac{1}{2} \int_\Omega \mathbb{E}\left(|\bar{T}_{\boldsymbol{\theta}}(u) - u|^2 \right) d\bar{\mu}(u),\end{aligned}$$

where the last equality above is a consequence of Fubini's Theorem which follows from the measurability of the mapping $(u, \theta) \mapsto \bar{T}_\theta(u)$ that has been stated in Section 2.2.

Therefore, we have shown that

$$\int_\Theta \int_\Omega S_{g(\theta)} f_\theta(x) d\mu_\theta(x) d\theta \leq J(\bar{\mu}),$$

for any $f^\Theta \in L^1(\Theta, X)$ such that $\int_\Theta f_\theta(x) d\theta = 0$ for all $x \in \Omega$. This inequality implies that

$$J_{\mathcal{P}^*} \leq J(\bar{\mu}) = \frac{1}{2} \int_\Omega \mathbb{E}\left(|\bar{T}_{\boldsymbol{\theta}}(u) - u|^2 \right) d\bar{\mu}(u), \tag{5.8}$$

where $J_{\mathcal{P}^*}$ denotes the maximal value of the dual problem (4.2).

b) Let us recall that we have assumed that $g(\theta) > 0$ for any $\theta \in \Theta$. Now, for any $\theta \in \Theta$, we define the function

$$f_\theta(x) = -g(\theta) \left(\bar{\phi}_\theta(x) - \frac{1}{2}|x|^2 \right), \ x \in \Omega, \tag{5.9}$$

where $\bar{\phi}_\theta$ is the l.s.c. convex function introduced in Condition (5.4). First, Assumption ii) ensures that $f^\Theta = (f_\theta)_{\theta \in \Theta}$ belongs to $L^1(\Theta, X)$. Moreover, by Condition (5.4), one has that $\int_\Theta f_\theta(x) d\theta = 0$ for all $x \in \Omega$. For any $(x, \theta) \in \Omega \times \Theta$, let us now consider the function $F : \Omega \to \mathbb{R}$ defined by

$$F(y) = \frac{g(\theta)}{2}|x - y|^2 - f_\theta(y) = \frac{g(\theta)}{2}|x - y|^2 + g(\theta) \left(\bar{\phi}_\theta(y) - \frac{1}{2}|y|^2 \right), \ y \in \Omega.$$

Note that $F(y) = \frac{g(\theta)}{2}|x|^2 - g(\theta)\langle x, y\rangle + g(\theta)\bar{\phi}_\theta(y)$. Hence, F is a convex function, since, by assumption, $\bar{\phi}_\theta$ is convex. Searching for some $y \in \Omega$, where the gradient of F vanishes, leads to the equation

$$0 \quad = \quad -g(\theta)(x-y) + g(\theta)\left(\nabla\bar{\phi}_\theta(y) - y\right) = -g(\theta)(x-y) + g(\theta)\left(\bar{T}_\theta(y) - y\right).$$

Since $g(\theta) > 0$, it follows that the convex function $y \mapsto F(y)$ has a minimum at $y = \bar{T}_\theta^{-1}(x) \in \Omega$. Therefore,

$$S_{g(\theta)}f_\theta(x) \quad = \quad \frac{g(\theta)}{2}|x - \bar{T}_\theta^{-1}(x)|^2 + g(\theta)\left(\bar{\phi}_\theta(\bar{T}_\theta^{-1}(x)) - \frac{1}{2}|\bar{T}_\theta^{-1}(x)|^2\right) \tag{5.10}$$

Let us introduce the notation $J^*\left(f^\Theta\right) = \int_\Theta \int_\Omega S_{g(\theta)}f_\theta(x)d\mu_\theta(x)d\theta$. By equation (5.10) and using the change of variable $u = \bar{T}_\theta^{-1}(x)$, one obtains that

$$\begin{aligned}
J^*\left(f^\Theta\right) &= \int_\Theta\int_\Omega \left(\frac{g(\theta)}{2}|x - \bar{T}_\theta^{-1}(x)|^2 + g(\theta)\left(\bar{\phi}_\theta(\bar{T}_\theta^{-1}(x)) - \frac{1}{2}|\bar{T}_\theta^{-1}(x)|^2\right)\right) d\mu_\theta(x)d\theta \\
&= \int_\Theta\int_\Omega \left(\frac{g(\theta)}{2}|\bar{T}_\theta(u) - u|^2 + g(\theta)\left(\bar{\phi}_\theta(u) - \frac{1}{2}|u|^2\right)\right) d\bar{\mu}(u)d\theta \\
&= \int_\Theta\int_\Omega \frac{g(\theta)}{2}|\bar{T}_\theta(u) - u|^2 d\bar{\mu}(u) = \frac{1}{2}\int_\Omega \mathbb{E}\left(|\bar{T}_{\boldsymbol{\theta}}(u) - u|^2\right) d\bar{\mu}(u)d\theta,
\end{aligned}$$

where the last equality follows as an application of Fubini's theorem combined with Condition (5.4). Hence, thanks to the upper bound (5.8), we finally have that

$$J^*\left(f^\Theta\right) = J_{\mathcal{P}^*} = \frac{1}{2}\int_\Omega \mathbb{E}\left(|\bar{T}_{\boldsymbol{\theta}}(u) - u|^2\right) d\bar{\mu}(u) = J(\bar{\mu}),$$

which proves that f^Θ is a maximizer of the dual problem $(\mathcal{P}^*)$. Moreover, by Proposition 4.1, one also obtains that that $J(\bar{\mu}) \leq J(\nu)$ for any $\nu \in \mathcal{M}_+(\Omega)$. Hence, $\bar{\mu} = \mu^*$ is the barycenter of the random measure $\mu_{\boldsymbol{\theta}}$. This completes the proof of Theorem 5.1. □

Theorem 5.1 shows that, under appropriate assumptions, computing the population barycenter in the Wasserstein space of the parametric random measure $\mu_{\boldsymbol{\theta}}$ amounts to transport the reference measure μ_0 by the expected amount of deformation measured by $\overline{T}$. We discuss below the Conditions (5.2), (5.3), and (5.4) stated in Theorem 5.1.

Condition (5.2) holds under appropriate assumptions on the smoothness of Ω, μ_θ and μ_0. Such assumptions may be difficult to summarize in a general setting. For a detailed review of sufficient assumptions ensuring that Condition (5.2) holds, we refer to the discussion in [18]. Nevertheless, in the next subsection, we provide various examples of statistical models for which such a condition holds.

In the case where $\overline{T} = I$ is the identity mapping, it can be checked that Conditions (5.3) and (5.4) are necessarily satisfied. Hence, if $\overline{T} = I$ and Condition (5.2) holds, then the population barycenter μ^* is equal to the reference measure μ_0. In this setting, the barycenter of the random measure $\mu_{\boldsymbol{\theta}}$ in the Wasserstein space is thus the measure μ_0 such that the expectation of the random optimal mapping $T_{\boldsymbol{\theta}}$ to push-forward $\mu_{\boldsymbol{\theta}}$ onto μ_0 is equal to the identity. In the next section, we illustrate this property deformable model of densities when using the Wasserstein metric to compare random distributions. Note that when $\overline{T} = I$, it is not required in Theorem

5.1 that the set of optimal maps $T_{\boldsymbol{\theta}}$ are admissible in the sense of Definition 4.2 in [15]. Indeed, according to this definition, a necessary condition for a countable collection of one-to-one maps $(T_\theta)_{\theta\in\Theta}$ to be an admissible class is that $T_\theta \circ T_{\theta'}^{-1}$ is an optimal mapping (in the sense of Proposition 2.1) for any $\theta, \theta' \in \Theta$. In the case where $\overline{T} = I$, such an assumption is thus not necessary.

When $\overline{T} \neq I$, Condition (5.3) is not necessarily satisfied since the composition $T_\theta \circ \bar{T}^{-1}$ between the optimal mapping T_θ and the map $\bar{T}^{-1}$ is not always an optimal mapping. In the following section, we describe statistical models to illustrate the usefulness of the barycenter in the Wasserstein space for data analysis, and we discuss various assumptions on $\overline{T}$ to ensure that Condition (5.3) is satisfied. Condition (5.4) is rather an identifiability condition. Indeed, by definition of $\overline{T}$, one always has that $\mathbb{E}(\bar{T}_{\boldsymbol{\theta}}(x)) = \int_\Omega \bar{T}_\theta(x) g(\theta) d\theta = x$ for all $x \in \Omega$. Hence, among the various convex functions $\bar{\phi}_\theta$ such that $\bar{T}_\theta = \nabla\bar{\phi}_\theta$, Condition (5.4) implies to choose the one that "integrates" the relation $\int_\Omega \bar{T}_\theta(x) g(\theta) d\theta = x$ without any additional constant term.

Finally, it should be also remarked that Condition (5.3) is weaker than requiring that $T_{\boldsymbol{\theta}} \circ T_{\boldsymbol{\theta}'}^{-1}$ is an optimal mapping for any $\boldsymbol{\theta}, \boldsymbol{\theta}' \in \Theta$. Therefore, even in the case where $\overline{T} \neq I$, the conditions stated in Theorem 5.1 to characterize a population barycenter by averaging optimal transport maps are weaker than those given in [15], since we do not require that the random optimal maps $T_{\boldsymbol{\theta}}$ belong to an admissible class of mappings (in the sense of Definition 4.2 in [15]). Moreover, we recall that the study in [15] is restricted to the characterization of empirical barycenters and their asymptotic properties.

6 An application to deformable models in statistics

In this section, we propose to discuss some applications of Theorem 5.1. To define probability models where averaging in the Wasserstein space amounts to take the expectation of an optimal transport map, we study statistical models for which the notion of population and empirical barycenters in the 2-Wasserstein space is relevant.

6.1 General framework

In many applications observations are in the form of a set of n one-dimensional signals or gray-level images $\mathbf{X}_1, \ldots, \mathbf{X}_n$ (e.g. in geophysics, biomedical imaging or in signal processing for neurosciences), which can be considered as iid random variables belonging to an appropriate space $\mathcal{F}(\Omega)$ of real-valued functions on a compact domain of $\Omega \subset \mathbb{R}^d$. In many situations the observed curves or images share the same structure. This may lead to the assumption that these observations are random elements which vary around a reference template. Characterizing and estimating such a template is then of fundamental interest in many applications.

In the presence of geometric variability in time or space in the data, a widely used approach is Grenander's pattern theory [25, 26, 40, 41] that models such a variability by the action of a Lie group on an infinite dimensional space of curves or images. Following the ideas of Grenander's pattern theory, a simple assumption is to consider that the data $\mathbf{X}_1, \ldots, \mathbf{X}_n$ are obtained through the deformation of the same template $h \in \mathcal{F}(\Omega)$ via the so-called deformable model

$$\mathbf{X}_i = h \circ \boldsymbol{\varphi}_i^{-1}, \ i = 1, \ldots, n, \tag{6.1}$$

where $\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_n$ are iid random variables belonging to the set of smooth diffeomorphisms of Ω. In signal and image processing, there has been recently a growing interest on the statistical analysis of deformable models (in the presence of additive noise) using either rigid or non-rigid random diffeomorphisms $\boldsymbol{\varphi}_i$, see e.g. [4, 11, 12, 13, 14, 23, 43] and the review proposed in [5]. Nevertheless, in a data set of curves or images, one generally observes not only a source of variability in geometry, but also a source of photometric variability (e.g. the intensity of a pixel changes from one image to another) that cannot be only captured by a deformation of the domain Ω via a diffeomorphism as in model (6.1).

It is always possible to transform the data $\mathbf{X}_1, \ldots, \mathbf{X}_n$ into a set of n iid random probability densities by computing the random variables

$$\mathbf{q}_i(x) = \frac{\widetilde{\mathbf{X}}_i(x)}{\int_\Omega \widetilde{\mathbf{X}}_i(u)du}, \ x \in \Omega, \ \text{where } \widetilde{\mathbf{X}}_i(x) = \mathbf{X}_i(x) - \min_{u\in\Omega}\left\{\mathbf{X}_i(u)\right\}, \ i = 1, \ldots, n.$$

Let $q_0 \in \mathcal{F}(\Omega)$ be a probability density function. In this section and as already discussed in the introduction, we consider the following deformable model of densities:

$$\mathbf{q}_i(x) = \left|\det\left(D\boldsymbol{\varphi}_i^{-1}\right)(x)\right| q_0\left(\boldsymbol{\varphi}_i^{-1}(x)\right) \ x \in \Omega, \ i = 1, \ldots, n, \tag{6.2}$$

where $\det\left(D\boldsymbol{\varphi}_i^{-1}\right)(x)$ denotes the determinant of the Jacobian matrix of the random diffeomorphism $\boldsymbol{\varphi}_i^{-1}$ at point x. If we denote by $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_n \in \mathcal{M}_+(\Omega)$ the random probability measures with densities $\mathbf{q}_1, \ldots, \mathbf{q}_n$, and by μ_0 the measure with density q_0, then (6.2) can also be written as the following deformable model of measures

$$\boldsymbol{\mu}_i = \boldsymbol{\varphi}_i \# \mu_0, \ i = 1, \ldots, n. \tag{6.3}$$

In model (6.3), under appropriate assumptions on the random maps $\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_n$, computing the empirical barycenter in the Wasserstein space of the random measures $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_n$ leads to a consistent and meaningful estimator of the reference measure μ_0 and thus of the template q_0. In the rest of this section, we discuss some examples of model (6.3). The main contribution is to show how Theorem 5.1 can be used to characterise the population barycenter of random measures satisfying the deformable model (6.3).

6.2 A parametric class of diffeomorphisms

Let μ_0 be a measure on $\mathbb{R}^d$ having a density q_0 (with respect to the Lebesgue measure dx on $\mathbb{R}^d$) whose support is contained in a compact set $\Omega_{q_0} \subset \mathbb{R}^d$. We propose to characterise the population barycenter of a random measure $\boldsymbol{\mu}$ satisfying the deformable model $\boldsymbol{\mu} = \boldsymbol{\varphi}\#\mu_0$, for a specific class of random diffeomorphisms $\boldsymbol{\varphi} : \mathbb{R}^d \to \mathbb{R}^d$. Let $\mathbb{S}_d^+(\mathbb{R})$ be the set of positive definite $d \times d$ symmetric matrices with real entries. Let

$$\phi : (\mathbb{R}^p, \mathcal{B}(\mathbb{R}^p)) \to \left(\mathbb{S}_d^+(\mathbb{R}) \times \mathbb{R}^d, \mathcal{B}\left(\mathbb{S}_d^+(\mathbb{R}) \times \mathbb{R}^d\right)\right) \tag{6.4}$$

be a measurable mapping, where $\mathcal{B}(\mathbb{S}_d^+(\mathbb{R}) \times \mathbb{R}^d)$ is the Borel σ-algebra of $\mathbb{S}_d^+(\mathbb{R}) \times \mathbb{R}^d$. For $\theta \in \mathbb{R}^p$, we will use the notations

$$\phi(\theta) = (A_\theta, b_\theta), \ \text{with } A_\theta \in \mathbb{S}_d^+(\mathbb{R}), \ b_\theta \in \mathbb{R}^d,$$

and

$$T_\theta(x) = A_\theta x + b_\theta,\ x \in \mathbb{R}^d.$$

Since the matrix A_θ belongs to $\mathbb{S}_d^+(\mathbb{R})$, it is clear that T_θ is the gradient of the convex function

$$\phi_\theta(x) = \frac{1}{2} x' A_\theta x + b_\theta' x,\ \text{for } x \in \mathbb{R}^d.$$

Moreover, for any $\theta \in \mathbb{R}^d$, it follows that $T_\theta : \mathbb{R}^d \to \mathbb{R}^d$ is a C^1 diffeomorphism with inverse given by

$$T_\theta^{-1}(x) = A_\theta^{-1}\left(x - b_\theta\right),\ x \in \mathbb{R}^d.$$

Let $\Theta \subset \mathbb{R}^p$ be a compact set, and let $\boldsymbol{\theta} \in \mathbb{R}^p$ be a random vector with density g (with respect to the Lebesgue measure $d\theta$ on $\mathbb{R}^p$) having a support included in Θ. We propose to study the population barycenter in the Wasserstein space of the random measure $\mu_{\boldsymbol{\theta}}$ satisfying the deformable model:

$$\mu_{\boldsymbol{\theta}} = T_{\boldsymbol{\theta}} \# \mu_0. \tag{6.5}$$

The above equation may also be interpreted as a semi-parametric model of random densities, where $T_{\boldsymbol{\theta}}$ is the optimal mapping between μ_0 and $\mu_{\boldsymbol{\theta}}$. For any $\theta \in \Theta$ (not necessarily a random vector), we define $\mu_\theta = T_\theta \# \mu_0$. Since T_θ is a smooth diffeomorphism and μ_0 is a measure with density q_0 whose support is included in the compact set Ω_{q_0}, it follows that μ_θ admits a density q_θ on $\mathbb{R}^d$ given by

$$q_\theta(x) = \begin{cases} \det\left(A_\theta^{-1}\right) q_0\left(A_\theta^{-1}\left(x - b_\theta\right)\right) & \text{if} \quad x \in \mathcal{R}(T_\theta), \\ 0 & \text{if} \quad x \notin \mathcal{R}(T_\theta). \end{cases} \tag{6.6}$$

where $\mathcal{R}(T_\theta) = \{T_\theta(y), y \in \Omega_{q_0}\} = \{A_\theta y + b_\theta, y \in \Omega_{q_0}\}$. If we further assume that the mapping $\phi : \Theta \to \mathbb{S}_d^+(\mathbb{R}) \times \mathbb{R}^d$ is continuous, it follows that there exists a compact set $\Omega \subset \mathbb{R}^d$ such that $\mathcal{R}(T_\theta) \subset \Omega$ for all $\theta \in \Theta$. Thus, under this assumption, the random measure $\mu_{\boldsymbol{\theta}}$ takes its values in $\mathcal{M}_+(\Omega)$.

As a consequence of Theorem 5.1, one has the following result.

Corollary 6.1. *Assume that the mapping ϕ defined in (6.4) is continuous, and let $\Omega \subset \mathbb{R}^d$ be a compact set such that $\mathcal{R}(T_\theta) \subset \Omega$ for all $\theta \in \Theta$. If*

$$\mathbb{E}(A_{\boldsymbol{\theta}}) = I \ \text{and}\ \mathbb{E}(b_{\boldsymbol{\theta}}) = 0$$

where I is the identity matrix, then $\mu_0 = \mu^*$ is the population barycenter in the Wasserstein space of the random measure $\mu_{\boldsymbol{\theta}} \in \mathcal{M}_+(\Omega)$ satisfying the deformable model (6.5).

In the case where the condition $\mathbb{E}(A_{\boldsymbol{\theta}}) = I$ is not necessarily satisfied, we define, for any $\theta \in \Theta$, the following quantities

$$\bar{A}_\theta = A_\theta \bar{A}^{-1} \quad \text{and} \quad \bar{b}_\theta = b_\theta - A_\theta \bar{A}^{-1} \bar{b}, \tag{6.7}$$

where $\bar{A} = \mathbb{E}\left(A_{\boldsymbol{\theta}}\right)$ and $\bar{b} = \mathbb{E}\left(b_{\boldsymbol{\theta}}\right)$. For any $\theta \in \Theta$, we also define the mapping

$$\bar{T}_\theta(x) = T_\theta(\bar{T}^{-1}(x)) = \bar{A}_\theta x + \bar{b}_\theta,\ x \in \mathbb{R}^d,$$

where $\bar{T}(x) = \mathbb{E}(A_{\boldsymbol{\theta}})x + \mathbb{E}(b_{\boldsymbol{\theta}})$. To apply Theorem 5.1, it is necessary to assume that $\bar{T}_\theta$ is the gradient of a convex function, which means assuming that $\bar{A}_\theta = A_\theta \bar{A}^{-1}$ is a positive definite matrix. A sufficient condition to have this property is to assume that the product $A_\theta \bar{A}^{-1}$ is symmetric for any $\theta \in \Theta$, since the product of two matrices in $\mathbb{S}_d^+(\mathbb{R})$ is positive definite if and only if their product is symmetric (see e.g. [34]). Under such assumptions, it is then possible to apply Theorem 5.1 to obtain following result.

Corollary 6.2. *Assume that the mapping ϕ defined in (6.4) is continuous, and let $\Omega \subset \mathbb{R}^d$ be a compact set such that $\mathcal{R}(T_\theta) \subset \Omega$ for all $\theta \in \Theta$. If $A_\theta \bar{A}^{-1}$ is symmetric for any $\theta \in \Theta$, then*

$$\mu^* = \bar{T} \# \mu_0.$$

is the population barycenter in the Wasserstein space of the random measure $\mu_{\boldsymbol{\theta}} \in \mathcal{M}_+(\Omega)$ satisfying the deformable model (6.5).

7 Convergence of the empirical barycenter

Let us now prove the convergence of the empirical barycenter for the set of measures considered in this paper under Assumption 1 (i.e. that they are compactly supported). We recall that this assumption implies that the Wasserstein space $(\mathcal{M}_+(\Omega), d_{W_2})$ is compact. This is the key property that we use to study the convergence of the empirical barycenter.

Let $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_n$ be iid random variables in $\mathbb{R}^p$ with distribution $\mathbb{P}_\Theta$. Then, let us define the functional

$$J_n(\nu) \quad = \quad \frac{1}{n} \sum_{j=1}^{n} \frac{1}{2} d_{W_2}^2(\nu, \mu_{\boldsymbol{\theta}_j}), \ \nu \in \mathcal{M}_+(\Omega), \tag{7.1}$$

and consider the optimization problem: find an empirical barycenter

$$\bar{\boldsymbol{\mu}}_n \in \underset{\nu \in \mathcal{M}_+(\Omega)}{\arg\min}\, J_n(\nu), \tag{7.2}$$

Thanks to the results in [2], the following lemma holds:

Lemma 7.1. *Suppose that Assumption 2 holds. Then, for any $n \geq 1$, there exists a unique minimizer $\bar{\boldsymbol{\mu}}_n$ of $J_n(\cdot)$ over $\mathcal{M}_+(\Omega)$.*

Let us now give our main result on the convergence of the empirical barycenter $\bar{\boldsymbol{\mu}}_n$.

Theorem 7.1. *Suppose that Assumption 1 and Assumption 2 hold. Let μ^* be the population barycenter defined by (1.2), and $\bar{\boldsymbol{\mu}}_n$ be the empirical barycenter defined by (7.2). Then,*

$$\lim_{n \to +\infty} d_{W_2}(\bar{\boldsymbol{\mu}}_n, \mu^*) = 0 \ \textit{almost surely (a.s.)}$$

Proof. For $\nu \in \mathcal{M}_+(\Omega)$, let us define

$$\Delta_n(\nu) = J_n(\nu) - J(\nu).$$

The proof is divided in two steps. It follows standard arguments to obtain a strong law of large number for random variables belonging to compact metric spaces that can be found in [39]. Theorem 7.1 can be seen as a particular case of the general results in [39]. But in order to be self contained we include a detailed proof that is inspired by the arguments in [39]. First, we prove the uniform convergence to zero of Δ_n over $\mathcal{M}_+(\Omega)$. Then, we show that any converging subsequence of $\bar{\boldsymbol{\mu}}_n$ converges a.s. to μ^* for the 2-Wasserstein distance.

Step 1. For $\nu \in \mathcal{M}_+(\Omega)$, let us denote by $f_\nu : \mathcal{M}_+(\Omega) \to \mathbb{R}$ the real-valued function defined by

$$f_\nu(\mu) = \frac{1}{2} d^2_{W_2}(\nu, \mu).$$

Then, let us define the following class of functions

$$\mathcal{F} = \{f_\nu,\ \nu \in \mathcal{M}_+(\Omega)\}.$$

Let $\delta^2(\Omega) = \sup_{x\in\Omega}\{|x|^2\}$. Since Ω is compact, it follows that $\mathcal{F}$ is a class of functions uniformly bounded by $2\delta^2(\Omega)$ (for the supremum norm). Now, let $\nu, \mu, \mu' \in \mathcal{M}_+(\Omega)$. By the triangle reverse inequality

$$\begin{aligned} |f_\nu(\mu) - f_\nu(\mu')| &= \frac{1}{2}\left|d^2_{W_2}(\nu,\mu) - d^2_{W_2}(\nu,\mu')\right| \leq \sqrt{2}\delta(\Omega)\left|d_{W_2}(\nu,\mu) - d_{W_2}(\nu,\mu')\right| \\ &\leq \sqrt{2}\delta(\Omega) d_{W_2}(\mu,\mu'). \end{aligned}$$

The above inequality proves that $\mathcal{F}$ is an equicontinuous family of functions. Now, let $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_n$ be iid random vectors in $\mathbb{R}^p$ with density g, and let us define the random empirical measure on $(\mathcal{M}_+(\Omega), \mathcal{B}(\mathcal{M}_+(\Omega)))$

$$\mathbb{P}_g^n = \frac{1}{n}\sum_{i=1}^n \delta_{\mu_{\boldsymbol{\theta}_i}} = \frac{1}{n}\sum_{i=1}^n \delta_{\phi(\boldsymbol{\theta}_i)},$$

where δ_μ denotes the Dirac measure. It is clear that

$$\Delta_n(\nu) = \int_{\mathcal{M}_+(\Omega)} f_\nu(\mu) d\mathbb{P}_g^n(\mu) - \int_{\mathcal{M}_+(\Omega)} f_\nu(\mu) d\mathbb{P}_g(\mu).$$

Let $f : \mathcal{M}_+(\Omega) \to \mathbb{R}$ be a real-valued function that is continuous (for the topology induced by d_{W_2}) and bounded. Thanks to the mesurability of the mapping ϕ, one has that the real random variable $\int_{\mathcal{M}_+(\Omega)} f(\mu) d\mathbb{P}_g^n(\mu)$ converges a.s. to $\int_{\mathcal{M}_+(\Omega)} f(\mu) d\mathbb{P}_g(\mu)$ as $n \to +\infty$, meaning that the random measure $\mathbb{P}_g^n$ a.s. converges to $\mathbb{P}_g$ in the weak sense. Therefore, since $\mathcal{F}$ is a uniformly bounded and equicontinuous family of functions, one can use Theorem 6.2 in [37] to obtain that

$$\sup_{\nu\in\mathcal{M}_+(\Omega)} |\Delta_n(\nu)| = \sup_{f\in\mathcal{F}} \left| \int_{\mathcal{M}_+(\Omega)} f(\mu) d\mathbb{P}_g^n(\mu) - \int_{\mathcal{M}_+(\Omega)} f(\mu) d\mathbb{P}_g(\mu) \right| \to 0 \text{ as } n \to +\infty, \ a.s. \quad (7.3)$$

which proves the uniform convergence of Δ_n to zero over $\mathcal{M}_+(\Omega)$.

Step 2. By Lemma 7.1, there exists a unique sequence $(\bar{\boldsymbol{\mu}}_n)_{n\geq 1}$ of empirical barycenters defined by (7.2). Thanks to the compactness of the Wasserstein space $(\mathcal{M}_+(\Omega), d_{W_2})$, one can extract a

converging sub-sequence of empirical barycenters $(\bar{\boldsymbol{\mu}}_{n_k})_{k\geq 1}$ such that $\lim_{k\to+\infty} d_{W_2}(\bar{\boldsymbol{\mu}}_{n_k}, \bar{\boldsymbol{\mu}}) = 0$ for some measure $\bar{\boldsymbol{\mu}} \in \mathcal{M}_+(\Omega)$.

Let us now prove that $\bar{\boldsymbol{\mu}} = \mu^*$. To this end, let us first note that by the definition of $\bar{\boldsymbol{\mu}}_{n_k}$ and μ^* as the unique minimizer of $J_{n_k}(\cdot)$ and $J(\cdot)$ respectively, it follows that

$$\begin{aligned} \left|J(\bar{\boldsymbol{\mu}}_{n_k}) - J(\mu^*)\right| &= J(\bar{\boldsymbol{\mu}}_{n_k}) - J_{n_k}(\bar{\boldsymbol{\mu}}_{n_k}) + J_{n_k}(\bar{\boldsymbol{\mu}}_{n_k}) - J_{n_k}(\mu^*) + J_{n_k}(\mu^*) - J(\mu^*) \\ &\leq 2 \sup_{\nu\in\mathcal{M}_+(\Omega)} |\Delta_{n_k}(\nu)|, \end{aligned}$$

where we have used the fact that $J_{n_k}(\bar{\boldsymbol{\mu}}_{n_k}) - J_{n_k}(\mu^*) \leq 0$. Therefore, thanks to the uniform convergence (7.3) of Δ_n to zero over $\mathcal{M}_+(\Omega)$, one obtains that

$$\lim_{k\to+\infty} J(\bar{\boldsymbol{\mu}}_{n_k}) = J(\mu^*). \tag{7.4}$$

Therefore, using that

$$\begin{aligned} \left|J_{n_k}(\bar{\boldsymbol{\mu}}_{n_k}) - J(\mu^*)\right| &\leq \left|J_{n_k}(\bar{\boldsymbol{\mu}}_{n_k}) - J(\bar{\boldsymbol{\mu}}_{n_k})\right| + \left|J(\bar{\boldsymbol{\mu}}_{n_k}) - J(\mu^*)\right| \\ &\leq \sup_{\nu\in\mathcal{M}_+(\Omega)} |\Delta_{n_k}(\nu)| + \left|J(\bar{\boldsymbol{\mu}}_{n_k}) - J(\mu^*)\right|, \end{aligned}$$

one finally obtains by (7.3) and (7.4) that

$$\lim_{k\to+\infty} J_{n_k}(\bar{\boldsymbol{\mu}}_{n_k}) = J(\mu^*). \tag{7.5}$$

Since $|J_{n_k}(\bar{\boldsymbol{\mu}}) - J(\bar{\boldsymbol{\mu}})| \leq \sup_{\nu\in\mathcal{M}_+(\Omega)} |\Delta_{n_k}(\nu)|$, it follows by equation (7.3) that

$$\lim_{k\to+\infty} J_{n_k}(\bar{\boldsymbol{\mu}}) = J(\bar{\boldsymbol{\mu}}) \; a.s. \tag{7.6}$$

Moreover, for any $\epsilon > 0$, there exists $k_\epsilon \in \mathbb{N}$ such that $d_{W_2}(\bar{\boldsymbol{\mu}}_{n_k}, \bar{\boldsymbol{\mu}}) \leq \epsilon$ for all $k \geq k_\epsilon$. Therefore, using the triangle inequality, it follows that for all $k \geq k_\epsilon$

$$\begin{aligned} (J_{n_k}(\bar{\boldsymbol{\mu}}))^{1/2} &= \left(\frac{1}{n_k}\sum_{j=1}^{n_k} \frac{1}{2} d^2_{W_2}(\bar{\boldsymbol{\mu}}, \mu_{\boldsymbol{\theta}_j})\right)^{1/2} \\ &\leq \left(\frac{1}{n_k}\sum_{j=1}^{n_k} \frac{1}{2} d^2_{W_2}(\bar{\boldsymbol{\mu}}_{n_k}, \mu_{\boldsymbol{\theta}_j})\right)^{1/2} + \left(\frac{1}{n_k}\sum_{j=1}^{n_k} \frac{1}{2} d^2_{W_2}(\bar{\boldsymbol{\mu}}, \bar{\boldsymbol{\mu}}_{n_k})\right)^{1/2} \\ &\leq \left(\frac{1}{n_k}\sum_{j=1}^{n_k} \frac{1}{2} d^2_{W_2}(\bar{\boldsymbol{\mu}}_{n_k}, \mu_{\boldsymbol{\theta}_j})\right)^{1/2} + \frac{\epsilon}{\sqrt{2}}, \end{aligned}$$

and thus by equations (7.5) and (7.6), we obtain that

$$J(\bar{\boldsymbol{\mu}}) \leq \lim_{k\to+\infty} J_{n_k}(\bar{\boldsymbol{\mu}}_{n_k}) = J(\mu^*) \; a.s. \tag{7.7}$$

which finally proves that $\bar{\boldsymbol{\mu}} = \mu^*$ a.s. since μ^* is the unique minimizer of $J(\nu)$ over $\nu \in \mathcal{M}_+(\Omega)$.

Hence, any converging subsequence of empirical barycenters converges a.s. to μ^* for the 2-Wasserstein distance. Since $(\mathcal{M}_+(\Omega), d_{W_2})$ is compact, this finally shows that $(\bar{\boldsymbol{\mu}}_n)_{n\geq 1}$ is a converging sequence such that $\lim_{n\to+\infty} d_{W_2}(\bar{\boldsymbol{\mu}}_n, \mu^*) = 0$ a.s. which completes the proof of Theorem 7.1.

□

8 Beyond the compactly supported case

To conclude the paper, we briefly discuss the case of a random measure $\mu_{\boldsymbol{\theta}}$ with distribution $\mathbb{P}_\Theta$ whose support is not included in a compact set Ω of $\mathbb{R}^d$. In the one-dimensional case i.e. $d = 1$, let us denote by $F_{\mu_{\boldsymbol{\theta}}}$ its cumulative distribution function, and by $F^{-1}_{\mu_{\boldsymbol{\theta}}}$ its generalized inverse (quantile function). Provided that one can define the measure μ^* with quantile function $F^{-1}_{\mu^*}(y) = \mathbb{E}\left(F^{-1}_{\mu_{\boldsymbol{\theta}}}(y)\right)$ for all $y \in [0,1]$, it is expected that arguments similar to those used in the proof of Theorem 3.1 can be used to prove that μ^* is the unique population barycenter of the random measure $\mu_{\boldsymbol{\theta}}$ with distribution $\mathbb{P}_\Theta$.

The multi-dimensional case (i.e. $d \geq 2$) is more involved. Indeed, the arguments that we used to prove the main results of the paper for $d \geq 2$ strongly depend on the compactness assumptions on the support of the random measure $\mu_{\boldsymbol{\theta}}$ and on the set Θ to which the random vector $\boldsymbol{\theta}$ belong. Adapting these arguments for the extension of this paper to non-compactly supported measures is an interesting topic for future investigations.

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